Vortex macroscopic superpositions in ultracold bosons in a double-well potential

M. A. Garcia-March[1,2] and Lincoln D. Carr[1,3]
[1] *Department of Physics, Colorado School of Mines, Golden, CO, 80401, U.S.A.*
[2] *Department of Physics, University College Cork, Cork, Ireland and*
[3] *Universität Heidelberg, Physikalisches Institut, 69120 Heidelberg, Germany*

We study macroscopic superpositions in the orbital rather than the spatial degrees of freedom, in a three-dimensional double-well system. We show that the ensuing dynamics of N interacting excited ultracold bosons, which in general requires at least eight single-particle modes and $\mathcal{O}(N^7)$ Fock states for large N, is described by a surprisingly small set of many-body states. An initial state with half the atoms in each well, and purposely excited in one of them, gives rise to the tunneling of axisymmetric and transverse vortex structures. This process generates macroscopic superpositions only distinguishable by their orbital properties and within experimentally realistic times.

Orbital physics play a crucial role in many important phenomena, due to the combination of orbital degeneracy and anisotropy of the vibrational states, and its correlation to other attributes, like charge or spin. For example, in metal transition oxides it is key to understanding high-temperature superconductivity or colossal magnetoresistance [2]. Recent experiments paved the way for the exploration of their role in the physics of ultracold atoms in three dimensional (3D) optical lattices [3], where this degree of freedom can be separated from those of charge and spin, and is the origin of exciting properties, such as novel phases or supersolidity [4]. Despite the fact that ultracold atoms are a natural system for realizing macroscopic superposition (MS) states [1], these have not been experimentally demonstrated therein, in part due to the very short decoherence times for such states. In this Letter we propose a new kind of MS state with the potential for greatly increased decoherence times, a *vortex macroscopic superposition* (VMS), based purely on orbital angular momentum instead of spatial superpositions in a 3D double well (DW).

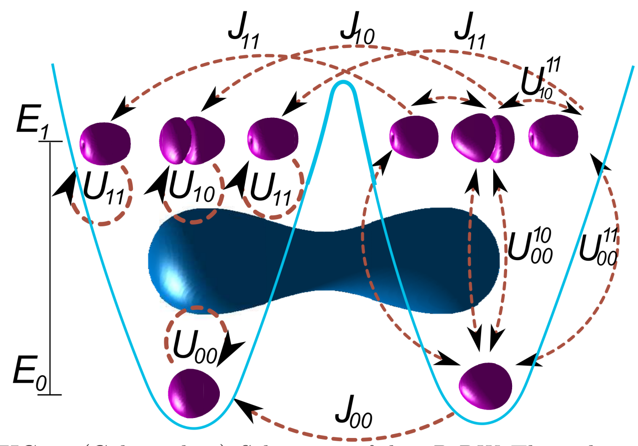

FIG. 1. (Color online) *Schematic of the 3D DW.* The eight orbital modes are represented as distorted spherical harmonics (magenta) and the processes among them by arrows. In the right well, the arrows represent both tunneling and interacting processes between different orbitals. The blue "peanut" shows the actual shape of an isoenergy surface of the DW.

Ultracold bosons in DWs are conventionally described by a two mode approach, accounting for the atoms condensed in the ground state and localized in either one of the two wells. If a great part of the population is intentionally excited to the first level of energies [3], the three degenerate orbital states localized at each well and showing z-component of the angular moment $m = -1, 0, 1$ have to be considered, together with new relevant processes, as sketched in Fig. 1 and discussed below. We assume that initially the atoms are distributed equally between both wells, and excited to an orbital state in one of them. Even though this eight-mode picture requires a great number of Fock states, we show that its dynamics is described by only a few many-body states. Then, while the number occupation of both wells remains constant under time evolution, the vortex tunnels between wells with a period shorter than the lifetime of a conventional experiment. This process is accompanied by the creation of VMSs. Spatial MSs decohere after a single interaction with an external particle. In contrast, VMSs must interact with many particles in order to spatially resolve the presence of the vortex on one side or the other, as external particles such as are found in the imperfect vacuum of experiments, as well as electromagnetic fields used to create the DW do not have a well-defined angular momentum; thus VMSs are stronger against decoherence than other MSs in DWs [5].

Ultracold bosons condensed in the ground state in DWs undergo two major processes: they interact in pairs in the same well with energy U or they can tunnel to the other well with energy J. The phenomena predicted by semiclassical mean field approaches, e.g., macroscopic quantum tunneling and self-trapping [6], were observed already in experiments [7]. Also, it has been shown that vortices can tunnel in DWs and that vortex-antivortex MSs can be obtained in a single trap [8]. Moreover, topological defects have attracted recently attention in connection to MSs [9], which in DWs are expected in the high barrier or *Fock regime* $NU \gg U \gg J$. In the Fock regime, mean field approaches cease to be useful, and other methods are required, with multiconfigurational Hartree methods the most numerically accurate techniques known to date [10], but impractical in the 3D

DW for VMSs. A simpler method based on direct diagonalization of Lipkin-Meshkov-Glick (LMG) like Hamiltonians with more than two modes is used in this Article, because it permits one to treat the 3D DW, to calculate with more atoms, and to obtain analytical results with perturbation techniques [11], as we will show.

Hamiltonian – A dilute gas of N ultracold bosons of mass M interacting through two-body interactions with coupling constant $g = 4\pi\hbar^2 a_s/M$, where a_s is the s-wave scattering length, is trapped in a 3D DW, which we assume is given by a separable potential $V(\mathbf{x})$, $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$, with harmonic 1D potentials in the x and y directions, and a Duffing potential in the z direction, $V(z) = V_0(-8z^2/a^2 + 16z^4/a^4 + 1)$. Since $V(\mathbf{x})$ takes the shape of a peanut with lobes in the z direction, as shown in Fig. 1, we call it the *peanut potential*. We consider a two-level eight single-particle mode expansion of the field operator in second quantization [12], giving $\hat{H} \equiv \sum_{\ell m} \hat{H}_{\ell m} + \hat{H}_{\rm int}$, with $\ell = 0, 1$ the level index and $\Delta E = E_1 - E_0$ the energy difference between levels. Here, $\hat{H}_{\ell m}$ are LMG Hamiltonians for each level:

$$\begin{aligned} H_{\ell m} &= U_{\ell m} \textstyle\sum_j \hat{n}_{j\ell m}(\hat{n}_{j\ell m} - 1) \\ &\quad - J_{\ell m} \textstyle\sum_{j' \neq j} \hat{b}^\dagger_{j\ell m} \hat{b}_{j'\ell m} + \sum_j E_\ell \hat{n}_{j\ell m}\,, \end{aligned} \tag{1}$$

where $\hat{n}^j_{j\ell m} = \hat{b}^\dagger_{j\ell m}\hat{b}_{j\ell m}$ is the number operator with well index $j = 1, 2$ for the left and right wells, respectively, level ℓ, and z component of the angular momentum m. Here $\hat{b}^\dagger_{j\ell m}$ and $\hat{b}_{j\ell m}$ are the creation/annihilation operators satisfying the usual bosonic commutation relations [12]. The interaction and tunneling coefficients for atoms with the same ℓ and m are $U_{\ell m}$ and $J_{\ell m}$, respectively (see Fig. 1). On the other hand $\hat{H}_{\rm int} = \hat{H}^m_{\rm inter} + \hat{H}_{\rm intra}$ is given by

$$\begin{aligned} \hat{H}^m_{\rm inter} &\equiv U^{1m}_{00} \textstyle\sum_j [(\hat{b}^\dagger_{j00})^2\, \hat{b}_{j1m}\hat{b}_{j1-m} + \text{h.c.}] \\ &\quad + 4\, U^{1m}_{00} \textstyle\sum_j \hat{n}_{j00}\, \hat{n}_{j1m}, \end{aligned} \tag{2}$$

$$\begin{aligned} &\hat{H}_{\rm intra} \equiv U^{11}_{10} \textstyle\sum_j [(\hat{b}^\dagger_{j10})^2 \hat{b}_{j11}\hat{b}_{j1-1} + \text{h.c.}] \\ &+ 2\, U^{11}_{10} \textstyle\sum_j \hat{n}_{j10}\,(\hat{n}_{j11} + \hat{n}_{j1-1}) + 2\, U^{11}_{11} \sum_j (\hat{n}_{j11}\hat{n}_{j1-1}). \end{aligned} \tag{3}$$

Equation (2) with $m = 0$ accounts for a *zero-vorticity interlevel hopping* process that permits two atoms in the ground state to be excited to an orbital with $m = 0$, or vice versa, with an energy U^{10}_{00}. For $m = \pm 1$, Eq. (2) accounts for a *vortex-antivortex interlevel annihilation and creation* process, in which two atoms are excited to (or decay from) an orbital with $m \neq 0$, each with a different sign of m, with energy U^{11}_{00}. Equation (3) accounts for a third process, *vortex-antivortex intralevel annihilation and creation*, in which two excited atoms with $m = 0$ can generate a pair of atoms with $m = \pm 1$ (each with different sign of m), or vice versa, with energy U^{11}_{10} (see Fig. 1). Notice that the 3D DW shows cylindrical symmetry with respect to the z axis, and two-fold ($\mathbb{Z}_2$) symmetry with respect to the x and y axis. Thus the z component of the angular momentum, $\mathbb{L}_z = \sum m\hat{n}_{j1m}$, is conserved. Conversely, the angular momentum operator $\mathbb{L}^2$, whose lengthy expression can be obtained for 3D DW using a conventional procedure [13], is not generally conserved.

We focus on the Fock regime, for which the interaction coefficients are much bigger than the tunneling ones, $\zeta_{\ell m} \equiv J_{\ell m}/U_{\ell m} \ll 1$, and we further assume that $\chi \equiv N \max_{\ell m \ell' m'} [U^{\ell' m'}_{\ell m}]/\Delta E \ll 1$, as is necessary for the eight mode single-particle approximation to be accurate [12]. We expand our states ψ in terms of the Fock basis, $|\psi\rangle = \sum_{i=0}^{\Omega} c_i |i\rangle$, where $\Omega = [(N+7)!]/[(N!)(7!)] \simeq N^7/7!$ for $N \gg 1$ is the dimension of the Fock space and $|i\rangle = \otimes_{j\ell m} |n^{(i)}_{j\ell m}\rangle$, with $|n^{(i)}_{j\ell m}\rangle = (n^{(i)}_{j\ell m})^{-1/2} (\hat{b}^\dagger_{j\ell m})^{n^{(i)}_{j\ell m}} |0\rangle$. We focus on the dynamics of vortex structures for zero population imbalance, i.e., the same number of atoms in each well. If all atoms remain in the lowest orbital, no tunneling process occurs. Conversely, if the atoms in one of the wells are excited to an orbital with the experimental techniques available [14], vortex structures tunnel between wells, accompanied with the creation of VMS states, as discussed below. There are two cases: (i) the vortex is *axisymmetric* and lies in the z-direction, i.e., $m = \pm 1$; and (ii) the vortex is *transverse*, lies in the $x - y$ plane, and $m = 0$. Other limiting cases, including non-zero population imbalance, are discussed in [13].

Case (i): Axisymmetric Vortex – The initial state is $|i\rangle$ with $n^{(i)}_{111} = N/2$ and $n^{(i)}_{200} = N/2$. We use high order perturbation theory to analyze the spectra of the two-level Hamiltonian, with the perturbing Hamiltonian the hopping terms in Eq. (1), and the interlevel Hamiltonian, Eqs. (2) and (3). We obtain quasidegenerate paired eigenvectors, $\psi = (1/\sqrt{2})(|i\rangle \pm |j\rangle)$, with $n^{(j)}_{211} = N/2$ and $n^{(j)}_{100} = N/2$, and splitting given by

$$\begin{aligned} &\Delta\varepsilon_{\pm 1} = 2(N/2!)^2 J_{00}^{N/2} J_{11}^{N/2} \tilde{U}\,, \\ &\tilde{U} = \sum_{i_1=0}^{1}\sum_{i_2=0}^{1}\cdots\sum_{i_{N-1}=0}^{1}\prod_{j=1}^{N-1} U\left(\sum_{k=1}^{j} i_k, j - \sum_{k=1}^{j} i_k\right), \\ &U(n,p) = (-1)^{(n+p)}\left\{U^{00}_{00} 2n[N/2 - n] + U^{11}_{11} 2p[N/2 - p]\right. \\ &\left. - 4U^{11}_{00}\,[N/2(n+p) - 2np]\right\}^{-1}, \end{aligned} \tag{4}$$

with $N/2 - 1 \leq \sum_{j=1}^{N-1} i_j \leq N/2$. We validated Eq. (4) for small N in simulations, and note that, despite the complex sums and lack of a simple expansion, the essential scaling is $\Delta\varepsilon_{\pm 1} \sim U^{00}_{00}(J_{00}J_{11})^{N/2}/N!(U^{00}_{00})^N$, since $U^{00}_{00} \sim U^{00}_{11} \sim U^{11}_{11}$ up to constant factors of order unity. In this case, the atoms slosh between wells with period $T = 2\pi\hbar/\Delta\varepsilon_{\pm 1}$, half of them always excited with $m = 1$, the other half non-excited, with occupation $\bar{n}_{j\ell m}(t) = \langle\psi(t)|\hat{n}_{j\ell m}|\psi(t)\rangle$ periodic for $\bar{n}_{111}$ and $\bar{n}_{200}$. The numerical calculations for these two variables via exact diagonalization are shown in Fig. 2(a),

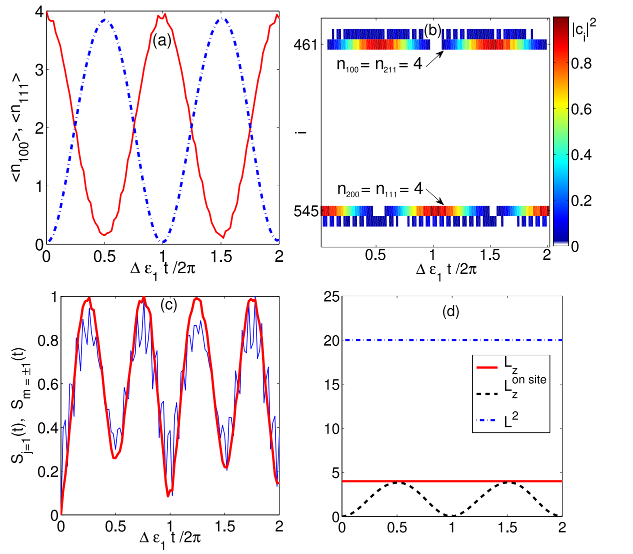

FIG. 2. (Color online) *Axisymmetric Vortex Tunneling.* (a) Average occupation of left well for unexcited, zero orbital angular momentum atoms (solid curve), and excited atoms in an axisymmetric vortex with $m = 1$ (dash-dotted curve). (b) Probability densities $P_i(t)$ showing the dominant Fock states i contributing to time evolution. The excited and unexcited atoms slosh between wells with the same period. (c) Spatial (solid thin curve) and angular momentum (solid thick curve) entanglement entropy. (d) Total $\mathbb{L}_z$ (solid curve) and total $\mathbb{L}^2$ (dash-dotted curve) are conserved, while on-site $\mathbb{L}_z$ (dashed curve) is not.

for $U_{00}^{00} = 1$, $\zeta_{00} = 1/5$, $J_{10}/J_{00} = 5$, $\chi = 1/10$. The probability $P_{111}(t)$ of finding $N/2$ excited atoms in well $j = 1$ with $m = 1$ and the probability $P_{200}(t)$ of them being non-excited in the other well are equal and given by $P_{111}(t) = P_{200}(t) = \cos^2(\Delta\epsilon_1 t/2\hbar)$. At the quarter period $P_{111}(t) = P_{200}(t) = 1/2$, and we obtain a VMS in the z-component of the angular momentum. Figure 2(b) plots the probability density in time, $|c_i(t)|^2$, showing that at $t = T/4$ the system is in a VMS. Since we consider only pure states, the VMS has zero total quantum entropy. However, the local entanglement or von Neumann entropy in space or angular momentum are both nonzero: the partial trace over the four modes in the right well, or alternately, over all modes but $\ell = 1, m = \pm 1$, yields algebraically complex expressions for $S_{j=1}$ and $S_{m=\pm 1}$, which we don't show here for brevity [13]. We normalize to the maximal entropy in each case and plot the results in Fig. 2(c). Both show a maximum at the quarter period, corresponding to the dynamical occurrence of the VMS. Finally, both total $\mathbb{L}^2$ and total $\mathbb{L}_z$ are conserved in this case. Conversely, on-site $\mathbb{L}_z$, obtained after restricting the index j to one of the wells, is not conserved and oscillates with period T.

Case (ii): Transverse Vortex – If the initial state $|i\rangle$ has $n_{110}^{(i)} = N/2$ and $n_{200}^{(i)} = N/2$, with N assumed even, the intralevel vortex-antivortex annihilation and creation process plays a crucial role, and pairs of atoms with $m = \pm 1$ can be created from pairs of excited atoms with $m = 0$.

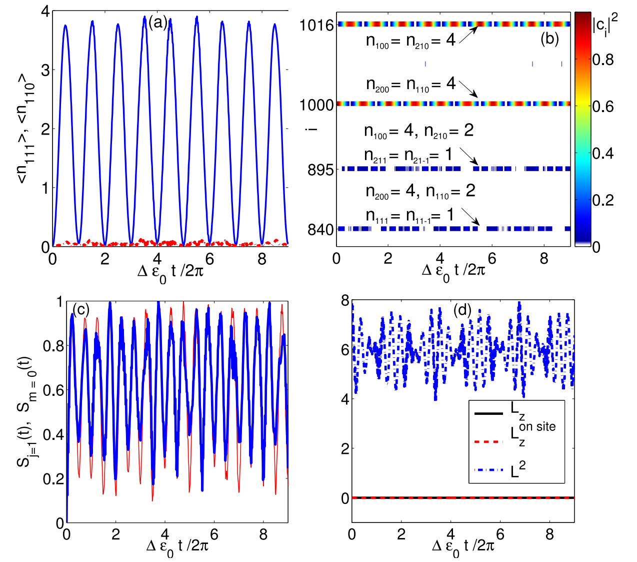

FIG. 3. (Color online) *Transverse vortex tunneling.* Panel layout as in Fig. 2. (a) Average occupation of left well for unexcited atoms (solid curve), and atoms in transverse vortex (dashed curve). (b) Four many-body modes now dominate, rather than just two – compare to Fig. 2. (c) Spatial (solid thin curve) and angular momentum (solid thick) entanglement entropy, here for $m = 0$. (d) Both total $\mathbb{L}_z$ (dashed curve) and on-site $\mathbb{L}_z$ (superposed) are conserved, while total $\mathbb{L}^2$ (solid curve) is not.

Using perturbation theory we find that the relevant Fock vectors include not only $|i\rangle$ and $|j\rangle$, but also, due to this process, two more vectors $|k\rangle$ and $|l\rangle$, where $n_{100}^{(j)} = N/2$ and $n_{210}^{(j)} = N/2$; $n_{100}^{(k)} = N/2$, $n_{210}^{(k)} = N/2 - 2$, and $n_{21\pm1}^{(l)} = 1$; and with $n_{200}^{(l)} = N/2$, $n_{110}^{(l)} = N/2 - 2$, and $n_{11\pm1}^{(l)} = 1$. Thus despite $\mathcal{O}(N^7)$ Fock vectors, the dynamics is described by combinations of just four of them, the quasidegenerate pairs $\psi_\pm = \alpha|i\rangle \pm \alpha|j\rangle + \beta|k\rangle \pm \beta|l\rangle$, with splitting $\Delta\varepsilon_0$, and $\phi_\pm = \mp\beta|i\rangle - \beta|j\rangle \pm \alpha|k\rangle + \alpha|l\rangle$, with splitting $\Delta\varepsilon_0'$. Perturbation theory shows that $\alpha \gg \beta$ and all other couplings to other Fock vectors are negligible [13]. We find the average number of particles in the right well in a transverse vortex state to be

$$\langle n_{200}\rangle = 2C(1 - \cos\Delta\varepsilon_0 t) + 2C'(1 - \cos\Delta\varepsilon_0' t)\,, \quad (5)$$

where $\hbar = 1$, $C = \alpha^2 N(\alpha^2 + \beta^2)$, $C' = \beta^2 N(\alpha^2 + \beta^2)$, and $C \gg C'$ since $\alpha \gg \beta$. In Fig. 3 we present, for this case, (a) the evolution of the average occupation of well $j = 1$ for excited atoms either with $m = 0$ or $m = 1$, and (b) of the probability density $P_i(t)$, when $U_{00} = 1$, $\zeta_{00} = 10^{-2}$, $J_{10}/J_{00} = 5$, $N = 8$, and $\chi = 1/10$. This four eigenvector problem leads to a quasiperiodic motion where the two relevant frequencies are proportional to the splittings, and where the modulation is very small due to the small coupling to Fock vectors with $n_{j1\pm1} = 1$. The local entanglement entropies $S_{j=1}$ and $S_{m=0}$, obtained from the partial trace over all modes but $\ell = 1, m = 0$, are shown in Fig. 3 (c). Now, the atoms tunnel between both wells with the same period, creating a transverse

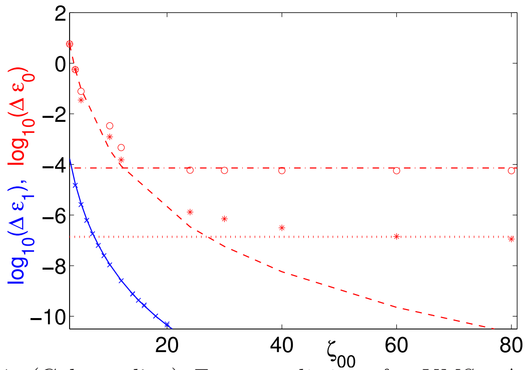

FIG. 4. (Color online) *Energy splittings for VMSs.* Axisymmetric (analytical: solid blue curve; numerical: blue crosses) and transverse (analytical: dashed, dotted, and dash-dotted red curves; numerical: red asterisks and circles) vortex cases. In the transverse case there are two limits: small and large $1/\zeta$. We represent the numerical results for $\chi = 1/80$ (asteriks) and $\chi = 1/10$ (circles). The analytical small $1/\zeta$ limit coincides in both cases (dashed curve). The analytical large $1/\zeta$ limit depends on ΔE and is represented as a dotted (dash-dotted) curve for $\chi = 1/80$ ($\chi = 1/10$).

VMS, and vortex-antivortex pairs are rapidly created and annihilated during this process. Finally, Fig. 3 (d) shows that, while $\mathbb{L}^2$ is not constant, both total and on-site $\mathbb{L}_z$ are conserved, since the atoms with $m = \pm 1$ are created in pairs.

The splittings can again be obtained using perturbation theory. There are two possible scenarios. First, if ζ_{00} is bigger than χ, the splitting will be given by Eq. (4) upon substitution of J_{11} by J_{10}, U_{11}^{11} by U_{10}^{10}, and U_{00}^{11} by U_{00}^{10}. Second, if ζ_{00} is much smaller than χ, the coupling between $|i\rangle$ and $|j\rangle$ is due to the zero-vorticity interlevel hopping. Then, this splitting is

$$\Delta\varepsilon_0' = 2(N/2)\,(N/2!)^2\,\left(U_{00}^{10}\right)^{N/2}\tilde{U}\,, \tag{6}$$
$$U(n,p) = \{U_{00}^{00}[4n(N/2-n) - 2n - 2p(2p-1)] +$$
$$U_{10}^{10}[4p(N/2-p-\frac{1}{2}) - 2n(2n-1)] + 2(p-n)\Delta E\}^{-1}\,,$$

with $\tilde{U}$ given in Eq. (4), i_j running only to $j = N/2-1$. Now, the essential scaling is $\Delta\varepsilon_0 \sim (N/2)!(U_{00}^{11})^{N/2}/N(N-1)\Delta E^{N/4}(U_{00}^{00})^{N/4-1}$. In Fig. 4 we show the splitting, both for the axisymmetric and transverse vortices, for $N = 8$ and different values of ζ_{00}. The axisymmetric splitting is smaller than the transverse splitting, and the analytical approach shows good agreement with the numerical calculation: thus transverse vortices tunnel faster; moreover, a transverse VMS is easier to make in experiments [14]. We also plot the analytical calculation for the splitting for the transverse vortex. First we use Eq. (4) as discussed above. The numerical calculation shows good agreement with this curve for small $1/\zeta_{00}$. For bigger values of this coefficient, the splitting tends to an asymptotic value, given by Eq. (6), which is increased for smaller values of χ.

Let us obtain the period of oscillation for typical experiments with $\omega = 2\pi \times 70$ Hz to 7 Khz with $\Delta E = \omega\hbar$. Taking $\chi = 1/2$ we obtain $U_{00}^{00} = \chi\Delta E/N = (0.125\,\text{to}\,12.5)\hbar$ Khz, which for $\zeta_{00} = 1/100$ gives $J_{00} = (1.25\,\text{to}\,125)\hbar$ Hz. For these quantities we obtain $\Delta\varepsilon \approx 7\,(10^{-3}\,\text{to}\,10^{-1})\hbar$ kHz, which gives a period of oscillation $T = 2\pi\hbar/\Delta\varepsilon = 1\,\text{to}\,0.01$ s, that is the oscillations will occur with a frequency of 1 to 100 Hz. MSs will be observable in an experiment if this time is shorter than the decoherence time. Conventional NOON states, where all atoms occupy simultaneously both wells, are extremely fragile against decoherence processes, such as those induced by imperfections of the potential [11], spontaneous emission, or the thermal cloud, among others [5], since they decohere after a single interaction. Since these sources of decoherence do not have a well-defined orbital angular momentum, VMS states have a much longer decoherence time: the core of the condensate has to be resolved by the environment to make the VMS collapse. The number of interactions is proportional to the total size of the condensate over the size of the core. For example, when the core occupies 1% of the total volume of the condensate, VMS decoherence time will be 100 times larger than for conventional MSs.

In conclusion, we have shown how vortex macroscopic superposition states arise from time evolution of vortex tunneling in a double well potential. Initial homogeneous distributions of atoms in both wells, excited in one of them to an orbital with $m = \pm 1$ (axisymmetric vortex) or with $m = 0$ (transverse vortex), give rise to the tunneling of the vortex structure, while the total average density remains constant in both wells. These VMS states are only distinguishable by their angular properties, and thus represent a new route for the realization of MSs with ultracold atoms in DW with potentially much longer decoherence times.

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